

Refining POWGEN data in TOPAS

Preamble

- TOPAS is a diffraction analysis package available in two versions; commercial with a GUI (Bruker-AXS) and academic without a GUI (<http://www.topas-academic.net/>).
- TOPAS doesn't 'know' about TOF data but may be used in versions 3 and above using the text-based launch-mode. This document assumes version 5 or 6.
- Launch-mode is very powerful, using something close to a computer code to create macros to manipulate/control the refinement in ways the developer never envisaged. Complex restraints, peak profiles, structure solution, rigid bodies, parametric and magnetic refinement are examples of what's possible within version 5. However the jump from the GUI mode in the commercial TOPAS to the more advanced features in launch-mode involves a steep learning curve.
- The TOPAS input file supplied from the POWGEN website is in the form of a template – no direct equivalent of the GSAS *.prm for Fullprof *.irf files exist. The template has been developed with version 5. It should be backwards compatible with version 4.2 and possibly version 3 but has not been tested.
- Template files from different cycles may be used interchangeably as long as correct calibration information for the relevant cycle (zero, difc, difa, alpha0, alpha1, beta0, beta1) is copied across. The template doesn't use the built-in TOF equations as it allows for more flexibility for future developments.
- The template files have been continually developed to improve their layout and add new functionality in the form of different customized macros. The template from 2016-B used here may look different from other cycles.
- Additional datasets such as lab/synchrotron X-ray or single-crystal may be added to these templates. Similarly Pawley, Le Bail and single-peak fitting can be done but the template was set up to simplify structure refinements of POWGEN data as much as possible.
- It is highly recommended that the jEdit text editor be used to work with the input files. Useful features such as color-coding, keyword menus, column editing and text-folding are available when set up correctly
- Information, TOPAS launch-mode tutorials and instructions for setting up jEdit for TOPAS can be found on the following website
https://community.dur.ac.uk/john.evans/topas_academic/topas_main.htm
- The TOPAS Technical Reference contains examples of the syntax and usage of the native TOPAS keywords/macros
- The TOPAS Wiki is a useful source of information, user-supplied macros and a user forum
<http://topas.dur.ac.uk/topaswiki/doku.php>

2016-B TOPAS Template structure – top half

The image shows a screenshot of a text editor window titled "jEdit - 2016B-60HR_PG3_btb_template.inp". The editor displays a template file with various sections and comments. The left sidebar shows a file tree with folders like "Xinsert", "TOPAS_Durham_Menu", "TOPAS_V5_Menu", "TOPAS_v3_Menu", "TOPAS_v4.1_Menu", "TOPAS_v4_Menu", and "Pam's TOPAS stuff".

Annotations in red text point to specific parts of the code:

- Green text denotes a comment started with ':** Points to the first line of the template: `'jEdit friendly TOPAS input file for POWGEN`
- Overall residuals and location for control commands:** Points to the section starting with `'Powgen 2016B calibration parameters`
- Section where filenames are entered:** Points to the section starting with `'{{{ select frames to use here and enter filenames [9 lines]`
- Frame-specific information and commands, e.g. scale factor:** Points to the section starting with `'{{{ information specific to frame 1 (0.533 WL) [27 lines]`
- Number of lines hidden by the fold:** Points to the fold indicator `[12 lines]` in the first fold.
- Fold indicator and expander:** Points to the left margin of the first fold.

The code content includes:

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1 'jEdit friendly TOPAS input file for POWGEN
2 'Back-to-back and positions as per GSAS-1 profile number 3
3 'number of possible broadening functions supported via macros in TOP_macros section at bottom of template
4 'built-in TOPAS TOF_CS_L and TOF_CS_G
5 'John Evans tof_sample_broadening
6 'GSAS-style sigmas and gammas can be calculated in POWGEN_instrument macro but no values supplied
7 'x-axis display in d-spacing and Q supported in version 6 - add the line " #define VERSION6 " in your local.inc file
8 'output of pattern simulation data in TOF, d and Q supported
9 'Folds used in file to allow for collapsing sections (in jEdit Utilities/Global options/Editing Folding-mode to explicit)
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12 'Powgen 2016B calibration parameters
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16 > {{{ i-factors and control information [12 lines]
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73 > {{{ information specific to frame 2 refinement here 1.066WL [28 lines]
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102 > {{{ information specific to frame 3 refinement here 1.333 [28 lines]
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132 > {{{ information specific to frame 4 refinement here 2.665 [28 lines]
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186 > {{{ information specific to frame 6 refinement here 4.797 [27 lines]
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```

2016-B TOPAS Template structure – bottom half

Menus to select different keywords

Overall structural information, lattice parameters, site information, etc

```
237 '-----
238 for xdds {
239   for strs 1 to 1 {
240     space_group "P"
241     phase_name ?
242     a ?
243     b ?
244     c ?
245     al ?
246     be ?
247     ga ?
248     site ?1 x ? y ? z ? occ ? 1.0 beq 0.3
249   }
250 }
251
252 ' add second phase here if needed for strs 2 to 2 () also needs second str info under each dataset used
253 '}}}
254 '}}}
255
256
257
258 '((( 'TOF macros
259 macro TOF_misc {
260   #ifdef VERSION6
261     gui_tof_t0 = zero;   gui_tof_t1 = dif_c; #endif
262     weighting = 1 / SigmaObs^2;
263     TOF_LAM(0.001)
264     scale_pks = D_spacing^4;
265     prm !two_theta 90
266
267 Abs_Lobanov 'absorption correction
268 TOF_d 'TOF to d-spacing
269 GSAS_btb 'back-to-back exponentials
270
271 macro TOF_d {
272   pk_xo = zero + dif_c D_spacing + dif_a D_spacing^2;
273 }
274 macro GSAS_btb
275 {
276   push_peak 'GSAS TOF peak shape 3
277   | exp_conv_const = alpha0 + alpha1 / D_spacing;
278   | bring_2nd_peak_to_top
279   | exp_conv_const = beta0 + beta1 / D_spacing^4;
280   | add_pop_1st_2nd_peak
281 }
282 }
283
284 macro Abs_Lobanov 'Lobanov absorption macro with calculated lambda for wavelength dependence of mu (as per GSAS manual)
285 {
286   prm !f 60.183 ' POWGEN 90 degree flightpath
287   prm !h_bar 6.626176e-34 ' Planck's constant
288   prm !m_n 1.67495e-27 ' neutron mass
289   prm !td_const = 10^4 h_bar/(m_n Lf);
290   local !sintheta = Sin(Deg_on_2 two_theta);
291   local !lambda = Xo 10^4 h_bar/(m_n Lf);
292   local !K0 = 1.697653;
293   local !K1 = (25.99978 - (0.01911 sintheta^0.5)Exp(-0.024514 sintheta^2)) + 0.109561 sintheta - 26.0456; 0.01578
294   local !K2 = -0.02489 - (0.39499 sintheta^2) + (1.219077 sintheta^3) - (1.31268 sintheta^4) + (0.871081 sintheta^5)
295     - (0.2327 sintheta^6);0.00535
296 }
```

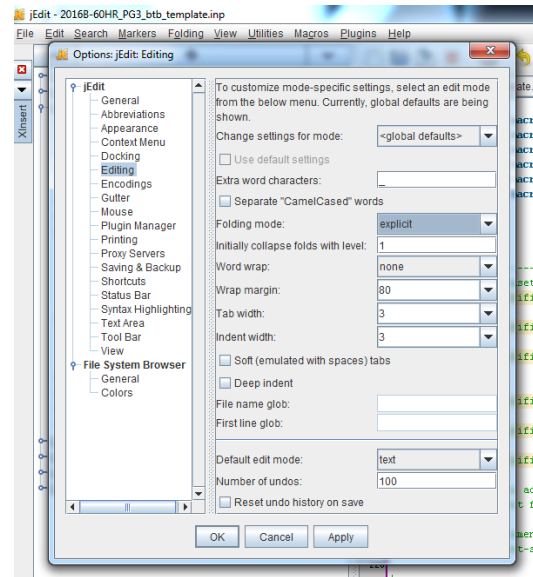
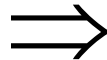
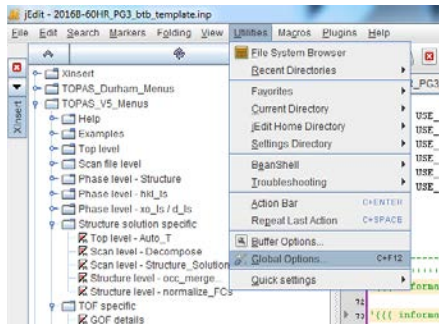
TOPAS has what it calls 'scope'.
"prm" declares a global variable
"local" declares a variable specific to the section and may have different values in different parts of the input file

Location of custom macros used within the template. DO NOT TOUCH UNLESS YOU ARE AN EXPERT! Changing anything may cause an error or even worse not cause an error potentially leading to incorrect results.

This is folded away and should not interfere with editing the rest of the input file

jEdit – folding

- Folding is a very useful feature, sections can be hidden away to simplify navigation of long text files.
- A fold is started by typing '{{{' and finished by '}}}'
- The text folding is not setup in the instructions given by John Evans' website but is easily set in the jEdit Global Options as shown by changing the Folding mode to 'explicit'



Refinements – initial setup

- Expand the section to add the required filenames

```
29
30 {{{ select frames to use here and enter filenames
31
32 #define USE_FRAME1 macro filename_frame1 {PG3_?-1.xye} macro start_end_frame1 {start_X 4800 finish_X 70000} '0.533 CWL
33 #define USE_FRAME2 macro filename_frame2 {PG3_?-2.xye} macro start_end_frame2 {start_X 6775 finish_X 104000} '1.066 CWL
34 #define USE_FRAME3 macro filename_frame3 {PG3_?-3.xye} macro start_end_frame3 {start_X 9930 finish_X 121700} '1.333 CWL
35 #define USE_FRAME4 macro filename_frame4 {PG3_?-4.xye} macro start_end_frame4 {start_X 26501 finish_X 207600} '2.665 CWL
36 #define USE_FRAME5 macro filename_frame5 {PG3_?-5.xye} macro start_end_frame5 {start_X 38400 finish_X 280000} '3.731 CWL
37 #define USE_FRAME6 macro filename_frame6 {PG3_?-6.xye} macro start_end_frame6 {start_X 51340 finish_X 346000} '4.797 CWL
38
39 }}}
40
41
```

Filenames, start and finish of data to fit in TOF for each frame

- Frames not required may either be commented out or deleted

```
--
30 {{{ select frames to use here and enter filenames
31
32 #define USE_FRAME1 macro filename_frame1 {PG3_?-1.xye} macro start_end_frame1 {start_X 4800 finish_X 70000} '0.533 CWL
33 #define USE_FRAME2 macro filename_frame2 {PG3_29601-2.xye} macro start_end_frame2 {start_X 6775 finish_X 104000} '1.066 CWL
34 #define USE_FRAME4 macro filename_frame4 {PG3_29603-4.xye} macro start_end_frame4 {start_X 26501 finish_X 207600} '2.665 CWL
35
36 }}}

```

```
16 {{{ r-factors and control information
17 r_exp      0.939678895
18 r_exp_dash 3.33349497
19 r_wp      4.30358706
20 r_wp_dash 15.2669023
21 r_p       5.54086233
22 r_p_dash  26.4086192
23 gof       4.57984859
24 weighted_Durbin_Watson 1.1501352
25 'continue_after_convergence
26 do_errors ←
27
```

Control information includes whether to calculate errors

Refinements – initial setup

- Sections relating unused frames may be deleted but will not cause an error when the refinement is run
- Expand a section in use, check parameters and add label to phase. Add 'view_structure' under the 'str' if you wish to see the structure during refinement

```
70 '({{ information specific to frame 2 refinement here 1.066WL
71 #ifdef USE_FRAME2
72 TOF_XYE(filename_frame2, = Yobs_dx_at(Xo) .5;) start_end_frame2
73 r_wp 0 r_exp 0 r_p 0 r_wp_dash 0 r_p_dash 0 r_exp_dash 0 weighted_Durbin_Watson 0 gof 0 'frame 2
74 bkg @ 0 0 0 0 0
75
76 local !zero -5.63852 'don't refine
77 local !dif_c 22572.52940 'don't refine
78 local !alpha0 64.48827 'don't refine
79 local !alphal -7.95180 'don't refine
80 local !beta0 42.83161 'don't refine
81 local !betal -0.63128 'don't refine
82
83 local !dif_a 0 'refine if necessary
84
85 local !mu 0 min 0 'refine if necessary
86 TOF_misc
87
88 str
89 phase_name ?
90 r bragg 0
91 scale scal_f2 1.52055946`_0.008257
92 peak_type pv
93 | TOF_CS_L(!cslf2, 200.57711, dif_c)
94 | TOF_CS_G(!csgf2, 72.35519, dif_c)
95 | tof_sample_peakshape(!lor_f2, 0.126077458,!dsp_f2, 15.34498,!dspsq_f2, 0.00000)
96
97 #endif
98 '}}}
```

Residuals for individual frame

Values for Chebychev polynomial background. User-defined background functions may be written when required

Diffractometer constants for this frame for particular cycle

Absorption coefficient

Calls different TOF macros (e.g. TOF to d-spacing, back-to-back peak shape, etc)

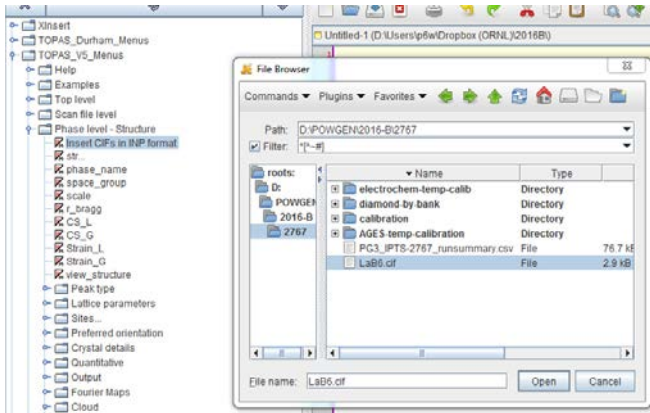
Scale factor

Peakshape parameters

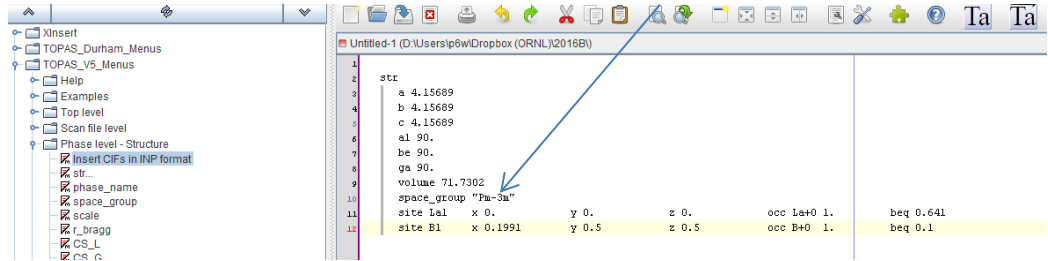
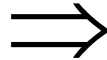
- Additional phases may be added by inserting another 'str'. Unless you want them to be constrained change the variable names for the scale, etc.

Adding structure information

- Structure information may either be typed in or imported from a CIF file. Beware – the jEdit CIF import occasionally needs two attempts to get the correct CIF file – make sure it's the right one



Some spacegroups have options for different origins (e.g. Fd-3m) but CIF files often don't specify which they used – CHECK!



- Correct any oddities from the CIF file, e.g. oxidation states, oxygens in water denoted by 'W', etc.
- Any special positions with recurring decimals much be declared as a fraction, e.g. "x 0.3333" should be "x = 1/3;" The ";" is important and must appear after any equation – without it TOPAS will probably throw an error but not always in the location where you expect!

```

235 for xdds {
236   for strs 1 to 1 {
237     str
238     a 4.15689
239     b 4.15689
240     c 4.15689
241     al 90.
242     be 90.
243     ga 90.
244     volume 71.7302
245     space_group "Fm-3m"
246     site La1 x 0.      y 0.      z 0.      occ La+0 1.      beq 0.641
247     site B1 x 0.1991  y 0.5     z 0.5     occ B+0 1.      beq 0.1
248   }
249 }
    
```

remove the 'str' statement

```

235 for xdds {
236   for strs 1 to 1 {
237     phase_name LaB6
238     a !lpa 4.15689
239     b =lpa;
240     c =lpa;
241     al 90.
242     be 90.
243     ga 90.
244     volume 71.7302
245     space_group "Fm-3m"
246     site La1 num_posns 0 x 0.      y 0.      z 0.      occ La 1.      beq 0.3
247     site B1 num_posns 0 x 0.1991  y 0.5     z 0.5     occ l1B 1.      beq 0.3
248   }
249 }
    
```

a parameter given variable name. "!" means it's fixed

Lattice parameters tied together with an equation.

TOPAS uses B_{iso} – not U_{iso}

"for xdds {}" and "for strs {}" loops tie together shared parameters from different datasets/structures.

IMPORTANT – DO NOT use "@" to set parameters to refine inside "for xdds {}" or "for strs {}" as it will create independent variables for each dataset and not do what you expect. Make up specific variables names, e.g. b_o, to ensure you get what you want.

"num_posns 0" will populate with site multiplicity after refinement

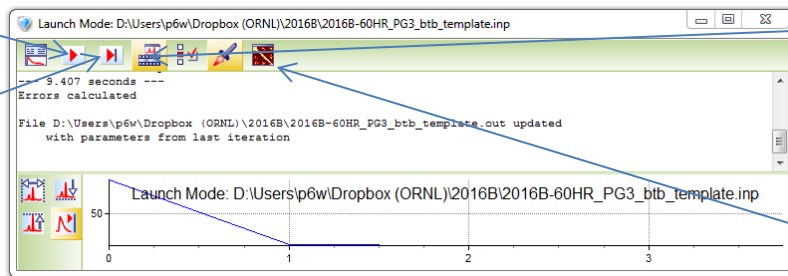
SRM-660b contains boron-11 isotope

Rerun refinement after convergence – if the real-time R_{wp} loops around each time around then probable that a '@' is in there somewhere..

Run the refinements...

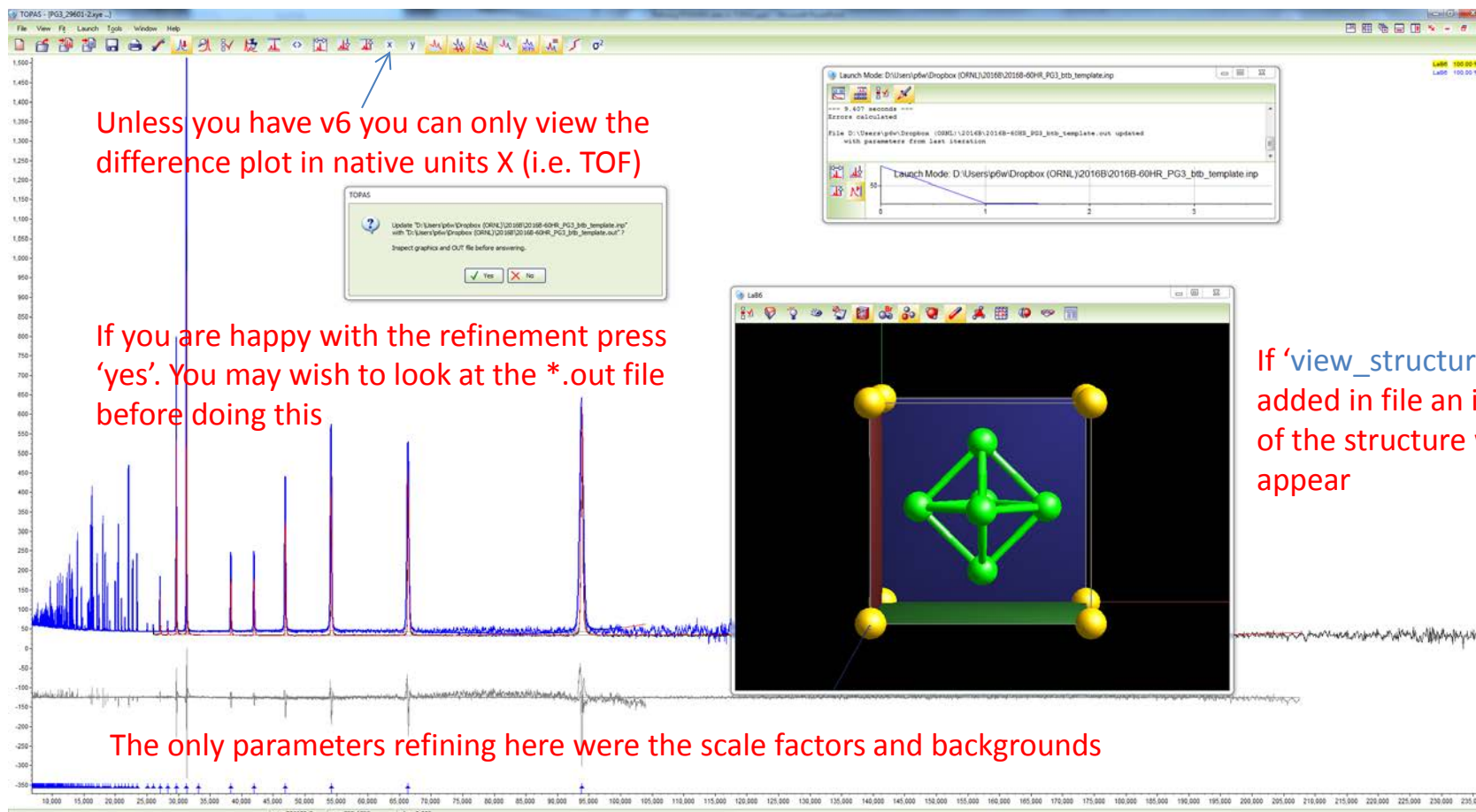
Run refinement to completion

Run refinement step-wise



Turns animation on and off.
Affects both difference plot and image of structure

If selected will display graphical representation of the correlation matrix (v5 and above)



Unless you have v6 you can only view the difference plot in native units X (i.e. TOF)

If you are happy with the refinement press 'yes'. You may wish to look at the *.out file before doing this

If 'view_structure' was added in file an image of the structure will appear

The only parameters refining here were the scale factors and backgrounds

Parameters pane...

- The parameters pane (F2 key or wrench button in interface) may be used to choose which dataset(s) to see in the main window.
- In the GUI mode this the main route to control and interact with the refinement, e.g. instrumental parameters, structure, microstructure, Pawley refinements....
- In launch-mode it is mostly inactive – the only useful pane under structures is the view of the generated hkl's under the structure. You may also customize the display of the difference plot in the parameters pane.

The screenshot shows the 'Parameters F2' window. On the left is a tree view with the following structure:

- Global
 - PG3_29601-2.xye
 - Emission Profile
 - Background
 - Instrument
 - Corrections
 - Miscellaneous
 - Structures/hkl Phases
 - LaB6
 - Sites
 - Preferred Orientation
 - Str Output
 - PG3_29603-4.xye

At the bottom left of the window, there are several menu items:

- Save Structure in STR format
- View/Hide Structure
- Create hkl's phase
- Delete Structure
- Paste INP to Node/Selections

On the right side of the window, there is a table with the following columns: Structure, Microstructure, Peak Type, hkl's, Additional Convolutions, and Rpt/Text. The table contains 18 rows of data.

Structure	h	k	l	m	d	th2	F ²
1	10	9	3	48	0.30157	6801.61572	9958.742
2	10	8	5	48	0.30237	6819.60059	4492.188
3	12	6	3	48	0.30237	6819.60059	109.143
4	11	8	2	48	0.30237	6819.60059	14601.884
5	13	4	2	48	0.30237	6819.60059	171.550
6	9	9	5	24	0.30398	6856.00195	4938.615
7	13	3	3	24	0.30398	6856.00195	3765.112
8	11	8	1	48	0.30480	6874.42236	1751.721
9	11	7	4	48	0.30480	6874.42236	3818.339
10	13	4	1	48	0.30480	6874.42236	4529.160
11	10	7	6	48	0.30562	6892.99219	4973.012
12	0	13	4	24	0.30562	6892.99219	2528.995
13	10	9	2	48	0.30562	6892.99219	1026.203
14	12	5	4	48	0.30562	6892.99219	9672.438
15	0	11	8	24	0.30562	6892.99219	741.427
16	12	6	2	48	0.30645	6911.71289	821.220
17	11	6	5	48	0.30813	6949.61670	372.317
18	10	9	1	48	0.30813	6949.61670	2452.741

Peak profiles...

- There are different options for fitting peak profiles in TOPAS. All of them assume a particular dependence with d-spacing. The two built-in functions are [TOF_CS_L](#) and [TOF_CS_G](#).

$$\text{FWHM}_{\text{lor}} = 0.1 \times \text{dffc} \times \text{d-spacing}^2 / \text{variable}_{\text{TOF_CS_L}}$$

$$\text{FWHM}_{\text{gauss}} = 0.1 \times \text{dffc} \times \text{d-spacing}^2 / \text{variable}_{\text{TOF_CS_G}}$$

- An alternative peak broadening function (written by John Evans) is supplied in the template that frequently does a better job of fitting peak profiles of POWGEN data. This is a macro called [tof_sample_peakshape](#) that is declared in the template itself that applies a pseudo-Voigt as follows

$$\text{FWHM}_{\text{lor}} = \text{lor} (\text{dsp} \times \text{d-spacing} + \text{dspsq} \times \text{d-spacing}^2)$$

$$\text{FWHM}_{\text{gauss}} = 1 - \text{lor} (\text{dsp} \times \text{d-spacing} + \text{dspsq} \times \text{d-spacing}^2)$$

- A macro called [POWGEN_instrument](#) is also described in the template TOF macros that follows uses GSAS-style sigmas and gammas. The sigma and gamma variables are not declared in the template as-supplied under the datasets but may be added by copy/paste with [POWGEN_instrument](#) to call the macro.

$$\text{FWHM}_{\text{lor}} = \sqrt{(\text{gam0} + \text{gam1} \times \text{d-spacing} + \text{gam2} \times \text{d-spacing}^2)^2}$$

$$\text{FWHM}_{\text{gauss}} = \sqrt{(\text{sig0} + \text{sig1} \times \text{d-spacing}^2 + \text{sig2} \times \text{d-spacing}^4)^2}$$

- Results of each profile function will vary depending on the particular sample
- The Stephens model for anisotropic strain broadening is either built-in (V5 and above) or available via the TOPAS wiki (V4.2 and below)
- More sophisticated models exist (see TOPAS wiki) but are frequently written for monochromatic radiation and may require modification for TOF

User-defined backgrounds

- The default Chebychev polynomial background function is frequently inadequate for high-Q TOF data due to oscillations caused by diffuse scattering.
- In V5 and above it is possible to write user-defined background functions via 'fit objects'.
- These may be written in TOF (X) or Q which may be defined for a dataset as
$$\text{local } Q = 2 \text{ Pi Constant(difc) / (X - Constant(zero));}$$
- One example of a user-defined background would be the diffuse scattering from positional disorder as described in the GSAS manual
- This has 3 refinable variables we'll call ba2, ba3 and sc1
- The fit object would be calculated as
$$\begin{aligned} \text{prm ba2 } &v1 \\ \text{prm ba3 } &v2 \\ \text{prm sc1 } &v3 \\ \text{Fit_obj !v1} &= \text{sc1 (Sin(Q ba2)/Q ba2) Exp(-0.5 ba3 Q^2);} \end{aligned}$$
- The fit object can then be plotted using
$$\text{Plot_Fit_Obj(v1, "Fit Obj1")}$$

Combined Neutron/X-ray refinements

- A space has been left in the template to allow the addition of another dataset, e.g. lab XRD or synchrotron dataset.
- The standard method of adding a XRD/constant wavelength dataset should be followed using a similar approach to the TOF data.
 - `xdd` filename.xxx loads the data
 - `bkg` uses a Chebychev background
 - `lam` is the wavelength
 - Lorentz polarization `LP_factor()`
 - `zero_error` for zero point correction
- XRD peakshape functions such as `CS_L()` should be used instead of TOF functions
- Should you wish to add a dataset from another TOF instrument (e.g. NOMAD) please contact one of the instrument team to correctly format the template

```
4 '({{ information specific to frame 6 refinement here 4.797
5 #ifdef USE_FRAME6
6 TOF_XYE(filename_frame6, = Yobs_dx_at(Xo) .5;) start_end_frame6
7 r_wp 0 r_exp 0 r_p 0 r_wp_dash 0 r_p_dash 0 r_exp_dash 0 weighted_Durbin_Watson 0 gof 0 'frame 6
8 bkg @ 0 0 0 0 0
9
10 local !zero -53.70751 'don't refine
11 local !dif_c 22600.51807 'don't refine
12 local !alpha0 -530.46172 'don't refine
13 local !alpha1 1219.01128 'don't refine
14 local !beta0 491.02832 'don't refine
15 local !beta1 -4362.10988 'don't refine
16
17 local !dif_a 0 'refine if necessary
18
19 local !mu 0 min 0 'refine if necessary
20 TOF_misc
21 str
22   phase_name ?
23   r_bragg 0
24   scale scal_f6 1
25   peak_type pv
26   TOF_CS_L(!cslf6, 580.50382, dif_c)
27   TOF_CS_G(!csgf6, 259.04919, dif_c)
28   tof_sample_peakshape(!lor_f6, 6.76091017e-008,!dsp_f6, 1.00000,!dspsq_f6, 2.36777)
29
30 #endif
31 {}}}
```

```
2
3 ' add information for additional dataset here, e.g. lab XRD, 11BM, etc
4 ' xdd ..... ' import file
5 ' bkg ...
6 ' lam ... 'instrument info
7 ' str .. 'dataset-specific structure info (scale, broadening, etc)
8
```

More advanced refinement.. ADPs

- As a refinement progresses different variables will need to be turned on and off with more sophisticated models applied.
- ADPs are used infrequently with powder X-ray data but are common with TOF neutron data.
- TOPAS is unusual in that it uses Bs for isotropic displacement parameters and Us for anisotropic displacement parameters (ADPs).
 - The relationship between B_{iso} and U_{iso} is: $U_{\text{iso}} = B_{\text{iso}}/8\pi^2$
- The correct syntax for refining ADPs may be created by running the macro `adps` for each required site.
- **Beware**
 - A bug crept into some versions of TOPAS where the correct site symmetry constraints for ADPs were not always created for some space groups; check Chapter 8.3 in Volume C of the International Tables if in doubt
 - The `adps` macro places the '@' refinement flag before the parameters which cannot be used safely inside a `for xdds` loop. Change the '@' for a unique variable name such as `u11_o1`.

ADPs and constraints

- Example is a refinement of corundum with 2016-B POWGEN data
- Unique variable names used for each refined U_{aniso}
- Constraints use the keyword `Get()` in equations to link parameters for the same site, e.g. in the oxygen site

`o_u12 = Get(u22)/2;`

- This gets the value of u22 for oxygen without specifying the variable name

```

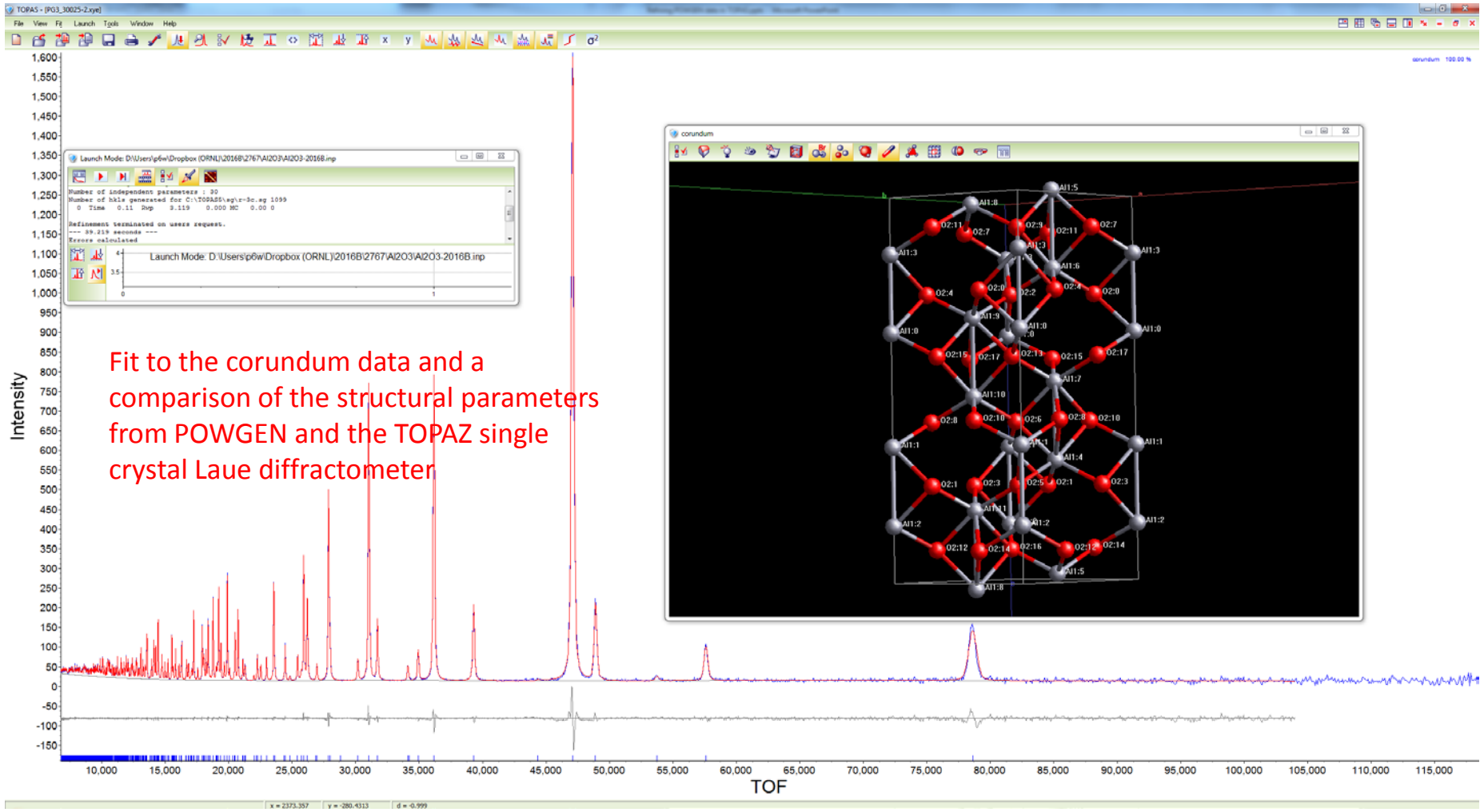
128 for xdds {
129   for strs 1 to 1 {
130     r_bragg 0.670561565
131     phase_name corundum
132     space_group R-3c
133     Trigonal(a_corundumori 4.760054`_0.000027 min =4.7400; max =4.7800;;c_corundumori 12.993475`_0.000087 min =12.9000; max =13.1000;)
134     site All num_posns 12 x =0; : 0.00000 y =0; : 0.00000 z z1_corundumori 0.35213`_0.00003 occ Al+3 1
135     ADPs { al_u11 0.00273`_0.00009 = Get(u11); al_u33 0.00299`_0.00012 al_u12 =Get(u11)/2;:0.00136`_0.00005 0 0 }
136     site O2 num_posns 18 x x2_corundumori 0.69363`_0.00003 y =0; : 0.00000 z =1/4; : 0.25000 occ O-2 1
137     ADPs { o_u11 0.00307`_0.00008 o_u22 0.00337`_0.00008 o_u33 0.00329`_0.00007 o_u12 =Get(u22)/2;:0.00169`_0.00004 o_u13 0.00025`_0.00003 =Get(u13)*2;:0.00050`_0.00005 }
138
139
140 }
141

```

- Symmetry check for R-3c. International Tables Volume C. Chapter 8.3 (uses β_{aniso} but same relationships)

Al = 12c with site symmetry '3.' $\beta_{11} = \beta_{22} = 2\beta_{12}; \beta_{13} = \beta_{23} = 0$

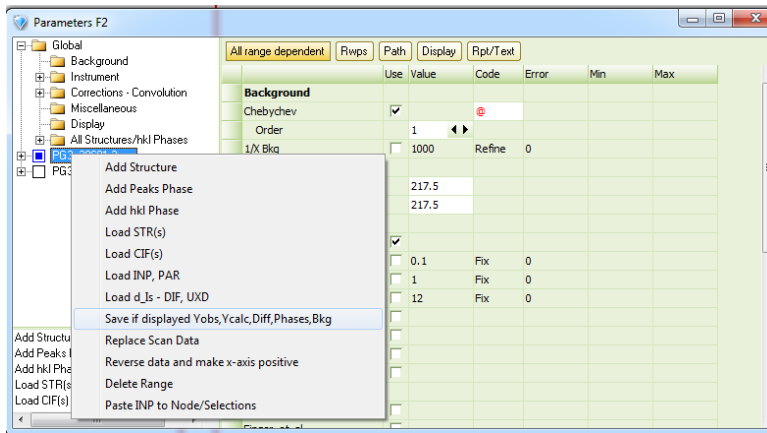
O = 18e with site symmetry '.2' $\beta_{22} = 2\beta_{12}; 2\beta_{13} = \beta_{23}$



	z (Al)	U11 (Al)	U33 (Al)	x (O)	U11 (O)	U22 (O)	U33(O)	U13 (O)
Laue single crystal neutron (GSAS)	0.35216(2)	0.00282(5)	0.00287(7)	0.30635(3)	0.00292(4)	0.00326(5)	0.00330(4)	
POWGEN (2016B)	0.35213(3)	0.00273(9)	0.00299(12)	0.30637(2)	0.00307(2)	0.00337(8)	0.00329(7)	0.00025(3)

Outputting data for publication...

- TOPAS 3/4 have very basic CIF output ([Out_CIF_STR](#)) but versions 5 and 6 have more sophisticated output built in for the structure ADPs ([Out_CIF_ADPs](#)), bond-lengths/angles ([Out_CIF_Bonds_Angles](#)), etc.
- Additional macros may be written to output the fit data in a format suitable for external plotting/publication – many can be found on the TOPAS Wiki.
- In version 5 and above fit data may be extracted from the parameters pane using “[Save if displayed Yobs, Ycalc, Diff, Phases, Bkg](#)”



Title	Description	Contributed by
Abs_Lobancv	Absorption correction for TOF neutrons	Pamela Whitefield
adp_no_limits	Remove positive definite limits on adps	Alan Coelho
Anisotropic_hkl	Anisotropic broadening correction based on the Alan Coelho reply in the Riet List on 31 Oct 2008	Carlos Pana-Santos and Selma G Antonio
Anisotropic_broadening	Anisotropic broadening correction based on an antiphase boundaries description by Her. Stephens et al	Emma McCabe and John S. O. Evans
Anisotropic_crystalite_size	Anisotropic broadening correction for triaxial-ellipsoids/elliptic-cylinders/cuboids	Dominique Ectors
DAC_Abs_Correction	Diamond anvil cell absorption correction	Martin Frisch
EoS_Macro	Determine equation of state parameters	Martin Etter and Robert E. Dinneber
FCF_Vesta	Shelx LIST 3 like FCF file for Vesta	Martin Frisch
gem_instrumental_peakshape	Gem tof peak shape	Bill David
Get_Distance_Get_Angle	Get the distance between two sites and report it in the .inp file	John Evans
H_side	Ride H atoms in organic structures	Alan Coelho
Inel_Flat_Plate_V1	Fixed sample angle I & disp. correct'n V1	Ian Madsen
Inel_Flat_Plate_V2	Fixed sample angle I & disp. correct'n V2	Ian Madsen
Insert_Peak	Add a peak to a Rietveld fit	John Evans
K-Factor	K-Factor Quantification	Martin Frisch
Out_CIF_crystalmaker	Output cif with adps for crystalmaker	John Evans
Out_CIF_ADPs_diamond	Cif with adps that diamond will read directly	Pamela Whitefield
Out_CIF_diamond	Cif with Diisos that diamond will read directly	Pamela Whitefield
Out_CIF_mag	Output magnetic CIF	John Evans and Emma McCabe
Out_Dif	Generate dif file in uxrd format for Bruker eva software	John Evans
Out_Gnuplot	Produce hkl labels and plots to use in gnuplot	John Evans
Out_min_max	Output coordinates in controllable formats	John Evans
Out_with_suffix	Versatile output for multipattern files	Martin Frisch
Out_xdl	Simple xdl format for various packages	John Evans
peak_shapes	Various peak shapes for various means	Matthew Rowles
Robust_refinement_xye	Robust Refinement	Peter Stephens
Stephens_peakshape	Anisotropic peak broadening	Peter Stephens
TOF_Powder_extinction	Extinction correction for TOF neutrons	Pamela Whitefield
tof_sample_peakshape	Sample contribution to tof peak shape	John Evans
wild_msc_wild_msc_new	tof peak shape GEM	Bill David
wild_peakshape	tof peak shape HRPD	Bill David
write_atoms	Write out coordinates for Atoms	John Evans
write_atoms_adp	Write atoms for .inp with adps for Atoms	John Evans
Bkg_GSAS_I2	Cosine fourier series background function (GSAS#2)	Pamela Whitefield
Out_GSAS_I2	Output coefficients for cosine fourier series (GSAS#2)	Pamela Whitefield
Bkg_GSAS_I5	GSAS background function #5 (low Q air-scatter)	Pamela Whitefield
Out_GSAS_I5	Output coefficients for GSAS background #5	Pamela Whitefield
Bkg_GSAS_I6	GSAS background function #6 (low Q air-scatter and high Q diffuse scattering)	Pamela Whitefield
Out_GSAS_I6	Output coefficients for GSAS background function #6	Pamela Whitefield

Pawley/Le Bail refinements

- Structureless cell refinements (Pawley and Le Bail) are easy to perform with TOPAS but the template was designed for Rietveld refinements and may require some modification.
- Pawley/Le Bail fits are triggered by using the keyword `hkl_Is` instead of `str`. Under `for xdds {}` the `for strs {}` will need changing to `for hklis {}`
- TOPAS will append the hkl list underneath the keyword `space_group`
- If `space_group` appears under `for xdds {}` and multiple frames are being fitted then the list from only the final dataset will be output.
 - In this instance move the `space_group` declaration to underneath each `hkl_Is` phase.
 - Remove or comment out redundant keywords such as the scale factor.
 - Fix absorption (`mu`) at zero
 - Remove or comment out all `site` lines under `hkl` or `for hklis {}`
- Pawley/Le Bail and Rietveld refinements can be combined in a single refinement but care must be taken to ensure everything is in the correct order under `for xdds {}`
- Note: POWGEN data can contain a very large number of reflections. Pawley refinements have individual position and intensity values for each reflection
 - The correlation matrix becomes extremely large so calculating errors with `do_errors` may take a very long time and use a lot of computing resources.

Pawley/Le Bail refinements

- Modified text required to switch to a Pawley refinement.
- To do a Le Bail refinement add the keyword
 lebail 1
under each **hkl_Is**

```
'{{{ information specific to frame 6 refinement here 4.797
#ifdef USE_FRAME6
TOF_XYE(filename_frame6, = Yobs_dx_at(Xo) .5); start_end_frame6
r_wp 0 r_exp 0 r_p 0 r_wp_dash 0 r_p_dash 0 r_exp_dash 0 weighted_Durbin_Watson 0 gof 0 'frame 6
bkg 0 0 0 0 0

local !zero -53.70751 'don't refine
local !dif_c 22600.51807 'don't refine
local !alpha0 -530.46172 'don't refine
local !alpha1 1219.01128 'don't refine
local !beta0 491.02832 'don't refine
local !beta1 -4362.10988 'don't refine

local !dif_a 0 'refine if necessary

local !mu 0 min 0 'refine if necessary
TOF_misc
hkl_Is
  phase_name ?
  r_braggy 0
  scale scal_f6 1
  peak_type pv
  TOF_CS_L(!csif6, 580.50382, dif_c)
  TOF_CS_G(!csgf6, 259.04919, dif_c)
  tof_sample_peakshape(!lor_f6, 6.76091017e-008,!dsp_f6, 1.00000,!dspsq_f6, 2.36777)
  space_group "?"
#endif
'')}}

' add information for additional dataset here, e.g. lab XRD, 11BM, etc
'xdd .... ' import file
'bkg ...
'lem ... 'instrument info
'str .. 'dataset-specific structure info (scale, broadening, etc)

-----

'{{{ overall structural information here
-----

'Put overall structural and peak shape information here
'Put the overall peak shape here so it can be refined for all banks in calibration then fixed for all banks
-----

for xdds {
for hklis 1 to 1 {
  space_group "?"
  phase_name ?
  a ?
  b ?
  c ?
  al ?
  be ?
  ga ?
  'site ?1 x ? y ? z ? occ ? 1.0 beq 0.3
}
}

' add second phase here if needed for str 2 to 2 {} also needs second str info under each dataset used
'')}}}
```